

Spin-polarized current in non-collinear antiferromagnets Mn_3X ($X = \text{Ga}, \text{Ge}, \text{Sn}, \text{Rh}, \text{Ir}, \text{Pt}$)

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Noncollinear antiferromagnets, such as Mn_3Sn and Mn_3Ir , were recently shown to be analogous to ferromagnets in that they have a large anomalous Hall effect. Here we show that these materials are similar to ferromagnets in another aspect: the charge current in these materials is spin-polarized. In addition, we show that the same mechanism that leads to the spin-polarized current also leads to a transversal spin current, which has a distinct symmetry and origin from the conventional spin Hall effect. We illustrate the existence of the spin-polarized current and the transversal spin current by performing *ab initio* microscopic calculations and by analyzing the symmetry. Based on the spin-polarized current we propose an antiferromagnetic tunneling junction, analogous in functionality to the magnetic tunneling junction.

Introduction. Spintronics is a field that studies phenomena in which both spin and charge degree of electron play an important role. Many of the key spintronics effects are based upon the existence of spin currents. Two main types of spin currents are utilized: the spin-polarized currents in ferromagnets (FMs) and the spin currents due to the spin Hall effect (SHE) which are transversal to the charge current and appear even in non-magnetic materials. The most important effects that originate from the spin-polarized currents in FMs are the giant and the tunneling magnetoresistance effects (GMR and TMR) [1–3] and the spin-transfer torque (STT) [4, 5]. These effects are utilized in magnetic tunneling junctions (MTJs), which form the basic building block of a new type of solid state memory, the magnetic random access memory (MRAM) [6]. This memory is non-volatile and has speed and density comparable to the widely used dynamic random access memory. The SHE on the other hand is responsible (though other effects can contribute) for the spin-orbit torque (SOT) [7, 8] in multilayer heterostructures, which can be used for efficient and fast switching of FM layers. The SOT is now also being explored for use in MRAMs [9, 10].

While spintronics has traditionally focused on FM and non-magnetic materials, in the past few years also antiferromagnetic (AFM) materials have attracted a considerable interest. AFMs offer some unique advantages compared to FMs, but are much less explored (see reviews [11–13]). AFMs have a very fast dynamics, which allows for switching on ps timescale [14–16]. Furthermore, there exists a wide range of AFM materials, including many insulators and semiconductors, multiferroics [17] and superconductors [18]. Utilizing (and also studying) AFMs is difficult, largely because the magnetic order in AFMs is hard to detect and to manipulate. Recently, electrical detection [19–23] and manipulation of the AFM order has been demonstrated [23, 24], however, both detection and manipulation still remain challenging from a practical point of view.

In this work we study spin currents generated by electrical fields in AFMs with non-collinear magnetic orders. We consider AFMs with triangular coplanar magnetic configurations: the hexagonal Mn_3Ga , Mn_3Ge and Mn_3Sn , which have the magnetic structure shown in Fig. 1(a) [25] as well as cubic AFMs Mn_3Rh , Mn_3Ir , Mn_3Pt which have the structure shown in Fig. 1(b) [26]. For simplicity we focus primarily on Mn_3Sn and Mn_3Ir . The triangular AFMs have recently attracted attention because they were shown to have a large anomalous Hall effect (AHE) [27–30] as well as the magneto-optical Kerr effect [31], even though they have only a very small net magnetization (which is not the origin of these effects).

Spin currents have been studied in AFMs before. Just like in nonmagnetic materials, transversal spin-currents will occur in AFMs due to the SHE. This has been predicted theoretically [32–34] and experimentally observed [32, 35–37]. It was also recently demonstrated that both collinear [38] and non-collinear AFMs [33, 39–42] can generate a large SOT on FMs in AFM/FM heterostructures. While the origin of such a torque is not clear [41] it is known that in heavy metal/FM heterostructures, the SHE plays an important role [43, 44]. Here we show, that apart from the conventional SHE, which was theoretically studied in Ref. [34], a different kind of spin currents also exist in the non-collinear AFMs, which are similar to the spin currents that occur in FMs. These spin currents are distinguished from the conventional SHE by transformation under time-reversal. While SHE is even under time-reversal, the spin currents discussed here are odd, analogously to the spin currents in FMs. Like in FMs, the odd spin currents contain a component which is longitudinal (i.e., flowing in the same direction as the the charge current), or in other words the charge current in the non-collinear AFMs is spin-polarized. Unlike in FMs, however, the odd spin currents also contain a large transversal contribution. We demonstrate the existence of the odd spin currents by microscopic *ab initio* calculations and by exploring the symmetry. We show that—just like

the AHE—the odd spin currents are a consequence of a symmetry breaking caused by the non-collinear magnetic structure. Since the spin-polarized current in the non-collinear AFMs is analogous to the spin-polarized current in FMs, we propose that the GMR, TMR and the STT effects should be present. These effects could provide an efficient way for electrical manipulation and detection of the AFM order and in particular could be utilized in an AFM tunneling junction (AFMTJ).

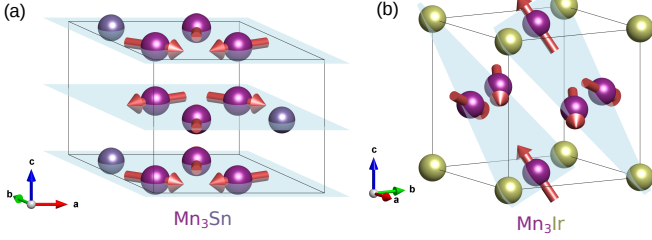


FIG. 1. (a) Crystal and magnetic structure of Mn₃Sn (as well as Mn₃Ga and Mn₃Ge) and (b) Mn₃Ir (as well as Mn₃Rh, Mn₃Pt).

Calculations. The response of metals to electric fields can be described well by linear response theory. Here we use the so-called constant Γ approximation, i.e., we assume that the only effect of disorder is a constant band broadening, which modifies the Green's functions of the perfectly periodic system in the following way: $G^R(\varepsilon) = 1/(\varepsilon - \hat{H} + i0+) \rightarrow 1/(\varepsilon - \hat{H} + i\Gamma)$, where \hat{H} is the Hamiltonian, ε is energy, G^R is the retarded Green's function (the advanced Green's function is modified analogously) and Γ is a constant that determines the broadening magnitude. Every linear response formula can be decomposed into two contributions which transform in the opposite way under time-reversal. Within the constant Γ approximation the two contributions to the linear response of an observable \hat{A} to an electric field are given by $\delta A = \chi^I E + \chi^{II} E$, where [44]

$$\chi^I = -\frac{e\hbar}{\pi} \sum_{\mathbf{k}, n, m} \frac{\Gamma^2 \text{Re} \left(\langle n\mathbf{k} | \hat{A} | m\mathbf{k} \rangle \langle m\mathbf{k} | \hat{\mathbf{v}} \cdot \hat{\mathbf{E}} | n\mathbf{k} \rangle \right)}{(E_F - \varepsilon_{n\mathbf{k}})^2 + \Gamma^2)(E_F - \varepsilon_{m\mathbf{k}})^2 + \Gamma^2}, \quad (1)$$

$$\chi^{II} = -2\hbar e \sum_{\substack{n \text{ occ.} \\ m \text{ unocc.} \\ \mathbf{k}, n \neq m}} \frac{\text{Im} \left(\langle n\mathbf{k} | \hat{A} | m\mathbf{k} \rangle \langle m\mathbf{k} | \hat{\mathbf{v}} \cdot \hat{\mathbf{E}} | n\mathbf{k} \rangle \right)}{(\varepsilon_{n\mathbf{k}} - \varepsilon_{m\mathbf{k}})^2}, \quad (2)$$

Here e is the (positive) elementary charge, \mathbf{k} is the Bloch wave vector, n, m are the band indices, $\varepsilon_{n\mathbf{k}}$ is the band energy, E_F is the Fermi energy, $\hat{\mathbf{v}}$ is the velocity operator, $\hat{\mathbf{E}}$ is the direction of the electric field and E its magnitude. In Eq. (2) the sum is restricted to m, n such that n is occupied and m is unoccupied. The sums over \mathbf{k} run over all \mathbf{k} points in the first Brillouin zone. We give

here the contribution χ^{II} only in the limit $\Gamma \rightarrow 0$, as this expression is usually considered in this limit. This contribution is known as the intrinsic contribution because it is determined only by the electronic structure of the perfect crystal. In the limit $\Gamma \rightarrow 0$, Eq. (1) becomes the well known Boltzmann formula with constant relaxation time (with the relaxation time given by $\hbar/2\Gamma$). This contribution is diverging as $1/\Gamma$ when $\Gamma \rightarrow 0$. While these formulas are simple they often provide at least qualitatively and sometimes even quantitatively correct description. They also correctly illustrate the symmetry of linear response. When \hat{A} is equal to current density operator: $\hat{\mathbf{j}} = -e\hat{\mathbf{v}}/V$, Eqs. (1), (2) describe conductivity. When \hat{A} is set to the spin-current operator, $\hat{j}_{i,j}^s = \frac{1}{2}\{\hat{s}_i, \hat{v}_j\}$, these equations instead describe spin-conductivity.

Eqs. (1) and (2) transform differently under time-reversal because time-reversal is an anti-unitary operator, which transforms the matrix elements as: $\langle n\mathbf{k} | \hat{A} | m\mathbf{k} \rangle \rightarrow \langle n\mathbf{k} | T \hat{A} T | m\mathbf{k} \rangle^*$ [45]. Because of the complex conjugation the term (2) will contain additional minus under a time-reversal transformation compared to the term (1). Thus for conductivity the term (1) is even under time-reversal, while the term (2) is odd. The even part describes the ordinary conductivity, while the odd part describes the AHE. Since AHE is odd under time-reversal it can be nonzero only in a nonmagnetic system (assuming non-interacting electrons). Traditionally, it has been considered for FMs only, but recently it was shown that Eq. (2) is also nonzero and relatively large in non-collinear AFMs [27, 28]. Collinear AFMs are typically symmetrical under simultaneous time-reversal and lattice translation or under simultaneous time-reversal and inversion and these symmetries prohibit the existence of AHE. In non-collinear AFMs, both of these symmetries are usually broken and thus the non-collinear AFMs can in general have an AHE.

For spin-conductivity the transformation under time-reversal is precisely opposite because the spin current operator contains an additional spin operator which is odd under time-reversal. Thus for spin-conductivity, Eq. (1) is odd under time-reversal, while Eq. (2) is even. The spin-currents that are even under time-reversal are known as the SHE. The odd spin-currents were previously considered only in FMs, however, as we will show in this manuscript they also exist in non-collinear AFMs (while in collinear AFMs they will typically be prohibited by the same symmetries as AHE), in complete analogy to the AHE. Since the intrinsic contribution to the spin currents in the triangular AFMs was recently explored in detail in [34], we focus here only on the spin-currents that are odd under time-reversal described by Eq. (1). To evaluate this equation, the ground state eigenvalues and eigenfunctions are needed, which we obtain from a non-collinear density functional theory calculation. We use the VASP code with the PBE-GGA exchange-correlation potential. To make the calculation faster we utilize the

		no SOC	SOC
Mn ₃ Sn	σ^x	$\begin{pmatrix} 0 & \sigma_{xy}^x & 0 \\ \sigma_{xy}^x & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}$	$\begin{pmatrix} 0 & \sigma_{xy}^x & 0 \\ \sigma_{yx}^x & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}$
	σ^y	$\begin{pmatrix} -\sigma_{xy}^x & 0 & 0 \\ 0 & \sigma_{xy}^x & 0 \\ 0 & 0 & 0 \end{pmatrix}$	$\begin{pmatrix} \sigma_{yx}^y & 0 & 0 \\ 0 & \sigma_{yy}^y & 0 \\ 0 & 0 & \sigma_{zz}^y \end{pmatrix}$
	σ^z	$\begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}$	$\begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & \sigma_{yz}^z \\ 0 & \sigma_{zy}^z & 0 \end{pmatrix}$
Mn ₃ Ir	σ^x	$\begin{pmatrix} \sigma_{xx}^x & 0 & 0 \\ 0 & -\frac{\sigma_{xx}^x}{2} & 0 \\ 0 & 0 & -\frac{\sigma_{xx}^x}{2} \end{pmatrix}$	$\begin{pmatrix} \sigma_{xx}^x & \sigma_{xy}^x & \sigma_{xz}^x \\ \sigma_{yx}^x & \sigma_{yy}^x & \sigma_{yz}^x \\ \sigma_{zx}^x & \sigma_{xy}^x & \sigma_{yy}^x \end{pmatrix}$
	σ^y	$\begin{pmatrix} -\frac{\sigma_{xx}^x}{2} & 0 & 0 \\ 0 & \sigma_{xx}^x & 0 \\ 0 & 0 & -\frac{\sigma_{xx}^x}{2} \end{pmatrix}$	$\begin{pmatrix} \sigma_{yy}^y & \sigma_{yx}^y & \sigma_{yz}^y \\ \sigma_{xy}^y & \sigma_{xx}^y & \sigma_{xy}^y \\ \sigma_{yz}^y & \sigma_{yx}^y & \sigma_{yy}^y \end{pmatrix}$
	σ^z	$\begin{pmatrix} -\frac{\sigma_{xx}^x}{2} & 0 & 0 \\ 0 & -\frac{\sigma_{xx}^x}{2} & 0 \\ 0 & 0 & \sigma_{xx}^x \end{pmatrix}$	$\begin{pmatrix} \sigma_{yy}^z & \sigma_{yz}^z & \sigma_{yx}^z \\ \sigma_{yz}^z & \sigma_{yy}^z & \sigma_{yx}^z \\ \sigma_{xy}^z & \sigma_{xy}^z & \sigma_{xx}^z \end{pmatrix}$

TABLE I. Symmetry restricted form of the odd spin-conductivity tensors in Mn₃Sn and Mn₃Ir with and without SOC. For Mn₃Ir the tensors are given in the coordinate system shown in Fig. 1(b). For Mn₃Sn we use a cartesian coordinate system related to the coordinate system in Fig. 1(a) in the following way: $\mathbf{x} = \mathbf{a}$, $\mathbf{y} = (\mathbf{a} + 2\mathbf{b})/\sqrt{3}$, $\mathbf{z} = \mathbf{c}$.

Wannier interpolation[34, 44]; see the Supplemental Material for a detailed description of the method.

Within linear response we can describe the spin current using a spin-conductivity tensor σ_{jk}^i , such that $\sum_k \sigma_{jk}^i E_k$ is the spin current with spin-polarization along i and flowing in the direction j . In Table I we give the general form of the odd spin-conductivity tensors for Mn₃Sn and Mn₃Ir. These can be derived by considering all the symmetry operations and how they transform the spin-conductivity tensor [45–47]. These symmetry tensors presume the existence of SOC. We find that the spin currents in the triangular AFMs appear even without the SOC (note that this is also true for the SHE in Mn₃Sn as we will discuss in a separate manuscript). In absence of the SOC, the symmetry is higher because spin is then not coupled to the lattice directly. The symmetry restricted shape of the odd spin-conductivity tensors in absence of SOC is also given in Table I. These tensors can be derived by considering combination of symmetries of the nonmagnetic lattice with pure spin rotations and are in good agreement with our calculations. See the Supplemental Material for further details. As shown in Table I, the symmetry in absence of the SOC is much higher than with the SOC. Both in Mn₃Sn and in Mn₃Ir the σ_{jk}^i tensors have only one independent component without the SOC.

In Fig. 2(a),(b) we plot the dependence of the magnitude of the odd spin currents in Mn₃Sn and Mn₃Ir on

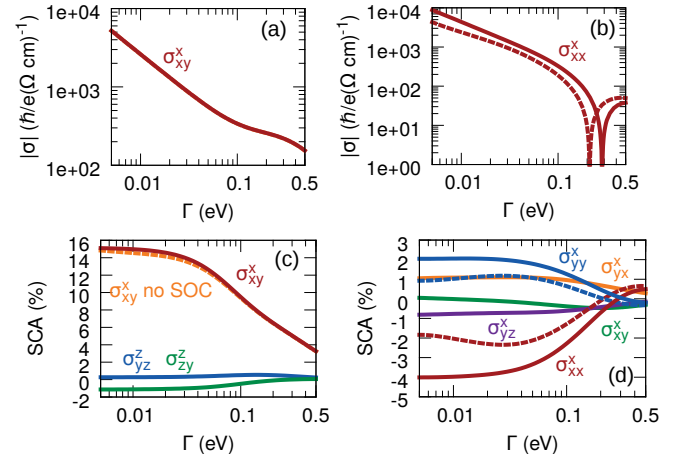


FIG. 2. Γ dependence of the odd spin currents in Mn₃Sn and Mn₃Ir. (a),(b) The magnitude of the spin current for Mn₃Sn and Mn₃Ir respectively. Only the largest component is shown for clarity. The dashed line denotes a calculation without SOC. The dip in (b) corresponds to a sign change. (c), (d) The SCA for Mn₃Sn and Mn₃Ir respectively.

Γ . As expected, for small Γ the odd spin currents are diverging as $1/\Gamma$. The magnitude of the SHE is often given in terms of the spin Hall angle, which is defined as $\frac{e}{\hbar} \frac{\sigma_{jk}^i}{\sigma_{kk}}$, where σ_{kk} is the conductivity [48]. Such quantity can be defined for any spin current. To distinguish it from the conventional spin Hall angle we call it the spin current angle (SCA). The SCA defined in this way is dimensionless. In Figs. 2(c),(d) we plot the SCA as a function of Γ for Mn₃Sn and Mn₃Ir. To evaluate the SCA we calculated the conductivity using Eq. (1). Since both the conductivity and the spin conductivity scale as $1/\Gamma$ for small Γ , the SCA is independent of Γ for small Γ .

We can estimate the value of Γ by comparing the calculated conductivity with the experimental conductivity. For Mn₃Ir the experimental conductivity at 300 K is $2.5 \times 10^4 (\Omega \cdot \text{cm})^{-1}$ [49]. This corresponds to $\Gamma \approx 0.05$ eV. For Mn₃Sn we find that even for very large values of Γ (up to 0.5 eV), the calculated conductivity is smaller than the experimental conductivity (see the Supplemental Material). This is probably because real crystals contain a significant amount of disorder, which cannot be captured by the constant Γ approximation.

In Table. II we give the calculated components of the spin-conductivity tensors for all the studied compounds. We set $\Gamma = 0.05$ eV in these calculations. We also give the calculated conductivity values for this Γ and the SCA for the longitudinal and transversal spin currents (denoted by α_{\parallel} and α_{\perp} respectively). As shown in Table. II, the odd spin currents are large in all the studied compounds. For comparison we calculated the odd spin currents in bcc Fe using the same method. We find that within the constant Γ approximation the longitudinal SCA in Fe is $\sim 18\%$ and the transversal SCA is $\sim 1\%$. Note that

	$\tilde{\sigma}_{xy}^x$	σ_{xy}^x	σ_{yx}^x	σ_{xx}^y	σ_{yy}^y	σ_{xx}	$\alpha_{ }$ (%)	α_{\perp} (%)	
Mn ₃ Ga	1503	1496	1490	-1511	1509	11022	13.7	13.5	
Mn ₃ Ge	229	252	249	-254	243	5009	5.1	5.0	
Mn ₃ Sn	564	559	566	-566	567	4571	12.4	12.4	
	$\tilde{\sigma}_{xx}^x$	σ_{xx}^x	σ_{yy}^x	σ_{xy}^x	σ_{yx}^x	σ_{yz}^x	σ_{xx}	$\alpha_{ }$ (%)	α_{\perp} (%)
Mn ₃ Rh	-123	-182	104	-80	19	-31	16002	1.1	0.7
Mn ₃ Ir	-496	-818	438	-56	265	-169	23647	3.5	1.9
Mn ₃ Pt	-999	-1029	469	-112	60	9	24575	4.2	1.9

TABLE II. Unique components of odd spin-conductivity tensors (in the units $\hbar/e(\Omega \cdot \text{cm})^{-1}$) in all the studied compounds for $\Gamma = 0.05$ eV. The σ_{zz}^y , σ_{yz}^y and σ_{zy}^y for Mn₃Ga, Mn₃Ge and Mn₃Sn are nonzero but small and are thus not given. $\tilde{\sigma}$ denotes a calculation without SOC. For each compound we also give the calculated conductivity (in the units of $(\Omega \cdot \text{cm})^{-1}$) and the SCA for the longitudinal current (denoted by $\alpha_{||}$) and for transversal spin-current (denoted by α_{\perp}).

such a calculation is only a rough estimate because the spin-dependent scattering is very important in FMs. As shown in Table II we find that in all the compounds, large spin currents are present even in absence of the SOC. In fact the SOC has a large effect only in Mn₃Ir.

Note that both Mn₃Sn and Mn₃Ir are not fully compensated, but have a small magnetic moment. Since this magnetic moment is very small, it cannot explain the odd spin currents discussed here. This is confirmed by calculation for Mn₃Ir in which the net magnetic moment is set to zero.

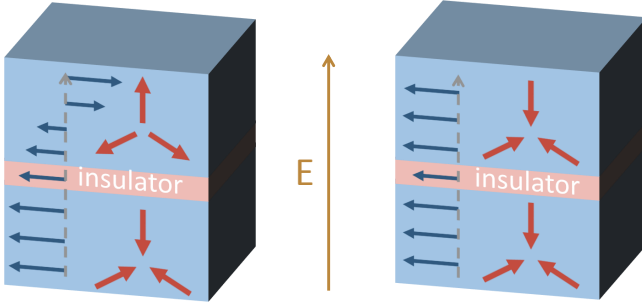


FIG. 3. AFM tunnel junction. Gray dashed arrow denotes direction of the spin current flow, blue arrows denote the spin polarization of the spin current and red arrows denote the magnetic moments.

Discussion. The spin currents discussed here are similar to the spin-polarized currents in FMs, but they differ in some aspects. In FMs, in absence of SOC, spin is a good quantum number and the current can be decomposed into a spin-up and spin-down currents. This is the so-called two current model. For non-collinear AFMs such description is not possible because in the presence of the non-collinear magnetic order, spin is not a good quantum number even without SOC.

In FMs, the origin of the spin-polarized current is easy to understand. The spin-up and spin-down electrons

that carry the current have different properties: there is a different number of spin-up and spin-down electrons at the Fermi level, the spin-up and spin-down electrons have different velocities (or alternatively different effective masses) and different scattering rates. Thus also the spin-up and spin-down currents will be different. In the non-collinear AFMs there is no spin-polarization at the Fermi level and we assume a spin-independent scattering rate, but the electrons with different spin can still have different velocities. In FMs, in absence of SOT, this mechanism leads only to longitudinal spin currents. In the non-collinear AFMs, as a consequence of their lower symmetry, it leads also to large transversal spin currents. Both of these spin currents could have important applications.

We first focus on the longitudinal spin currents. These spin currents are analogous to the spin-polarized currents in FMs and will thus have similar implications. One can imagine an AFMTJ, illustrated in Fig. 3, similar to the MTJ. Just like in MTJ, we can now consider two states of the AFMTJ: a parallel configuration in which both layers have the same directions of magnetic moments and an antiparallel configuration in which one layer has all the magnetic moments flipped. Since the spin currents discussed here are odd under time-reversal, in the antiparallel configuration the spin current in the second layer will have opposite spin-polarization compared to the spin current tunneling from the first layer. Conversely, in the parallel configuration, the spin current will have the same spin-polarization in both layers. This is completely analogous to the MTJ and thus we expect that both the TMR and the STT effects will be present (the STT will generally exist in presence of any non-collinear magnetic texture, such as a domain wall or an AFM skyrmion). Here we have focused on the tunneling junctions, however, we expect that the in a metallic junction the GMR effect will also be present. Compared to a MTJ, the AFMTJ would allow for much faster switching due to the inherently fast AFM dynamics and would be furthermore less sensitive to external magnetic fields and produce no stray fields. The calculated spin-polarized currents are relatively large, however, estimating the magnitude of the TMR and STT effects is beyond the scope of this work. Recently, it was shown that spin current injected into Mn₃Sn or Mn₃Ge can indeed control the magnetic order [50].

We note that there has been several proposals for an AFM junctions (tunneling or metallic) based on collinear AFMs [51–54], but so far only a tiny TMR effect has been demonstrated [55]. The non-collinear AFMTJs are promising candidates for an experimental realization of an AFMTJ since they are based on the same mechanism as the, experimentally well established, FM MTJs. We also remark that the longitudinal spin currents can occur in nonmagnetic materials as well if the crystalline symmetry is low enough [56]. Such spin currents differ from

the spin-polarized currents discussed here since they are even under time reversal and require SOC.

The transversal spin currents are similar to the spin currents due to the SHE, but they have a different symmetry properties. In particular, since these spin currents are odd under time-reversal, the spin currents in magnetic domains with opposite magnetic moments will be precisely opposite and thus the odd spin currents will tend to cancel out in samples with many magnetic domains. Recently several experiments have demonstrated a SOT in FM/Mn₃Ir heterostructures [33, 39, 41, 42]. While the origin of this torque is still discussed, it is generally assumed to be at least partly generated by the SHE. Since our calculations show that the odd transversal spin currents are in Mn₃Ir larger than the intrinsic SHE (the intrinsic SHE in Mn₃Ir is $215 \hbar/e(\Omega \cdot \text{cm})^{-1}$ [34]), we expect them to also contribute to the SOT.

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